Sandia National Laboratories

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Tracking# (SAND, PR) _____

Reactive Molecular Dynamics Simulations of Hot Spot Growth in Shocked Energetic Materials CCC8-133

U.S. DEPARTMENT OF ENERGY

SAND2015-7464R

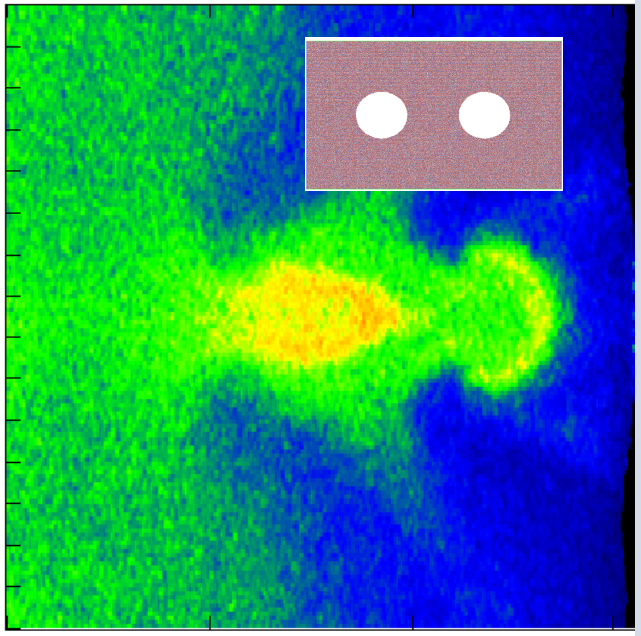
National Nuclear Security Administration

- Large-scale reactive molecular dynamics (MD) simulations of shock compression in energetic materials provide new insight in to the microscopic mechanisms leading up to detonation.
- Running LAMMPS on 16k nodes of Sequoia, we are able to run simulations with larger voids and multiple voids.
- In the most recent simulation containing 10 million atoms with two embedded 50nm voids, we have discovered that the hot spot intensity is much greater than for two non-interacting voids.

Principal Investigator: Aidan Thompson

Platform and Campaign ID: Sequoia
Usage: 4.2 days

Void-void Amplification



Temperature map from MD simulation of hot spot formation and growth around two 50nm voids in HNS taken 8 ps after the 1.25 km/s impact. Inset shows the pre-shock configuration.

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